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16. ABSTRACT

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On the Use of Indices in Aquatic Toxicological Hazard Assessment[1]

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Application of environmental indexing techniques to aquatic toxicological hazard assessment is illustrated, using three common data types (factors): acute invertebrate and vertebrate LC_{50} data and octanol–water partition coefficients for 37 chemical compounds. Subindex factor rating scales are constructed, total index computation is illustrated, and possible uses of this or other similar indices are discussed.

INTRODUCTION

Oftentimes decisions on the potential hazards of chemical introduction and use must proceed without the benefit of an in-depth hazard assessment for the substance in question. At this stage, relative hazard potential is of high concern, and there is usually uncertainty over whether *de novo* testing should be required. This paper discusses techniques that can aid in such preliminary assessments. The proposed techniques are not intended to preclude or obviate necessary test and assessment protocols designed to provide the more definitive information needed to estimate a compound's probable environmental effect.

Current chemical hazard assessment procedures are often complex and lack a common point of departure for consideration of aquatic toxicological effects. Such fundamental considerations as agreement on the types of required data and the processes for combining such data into a single assessment score seem to be lacking. Indexing—the process of scaling and combining disparate considerations (e.g., toxicity, accumulation, persistence data), into a single score—would appear to offer tangible benefits to the assessment process and the general problems of rapid identification of problem substances and the expression of relative toxicological properties of unknown or unstudied compounds. Most existing or proposed schemes appear to be unrealistically data-demanding; few attempt to perform assessments on the basis of existing or easily obtained information.

[1] Contribution No. 432, U. S. Environmental Protection Agency, Gulf Breeze, Fla.

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This paper attempts to review some of the problems inherent in toxicological hazard assessment, to establish semiquantitative procedures, and to make some preliminary evaluation of the proposed methodology. Although the index proposed here was originally designed to reflect aquatic toxicological concerns, the methods employed might be useful in other situations.

CURRENT ASSESSMENT PROCEDURES

Various assessment procedures or profiling proposals have been discussed in the literature, frequently with the recommendation that a test system or protocol be initiated. Several examples follow.

Beck *et al.* (1981) proposed a system for the evaluation of "new chemical" safety. Their proposed procedure departs from "prework" on available physical, chemical, and biological data to a decision to use or not use a chemical. They apply the method retrospectively, using examples. Potentially, indexing could aid in establishing a comparative basis at a number of places in their flow chart (Fig. 2, p. 21).

Korte *et al.* (1978) and Freitag *et al.* (1979) have proposed ecotoxicological profile and chemical screening techniques built around six factors: metabolism, bioaccumulation, photocatalysis, fate in sewerage, incineration, and waste composting. Their proposed system is unique in that it uses reference compounds, employs radiotracers, and allows "within"-factor rankings. However, widespread application of their system would require a large effort to test currently known chemical compounds. This technique depends entirely on the generation of new data and makes little use of existing physical, chemical, or biological information.

Portmann (1981) reported on a five-factor profiling procedure intended to evaluate the relative hazard of chemical substances carried by marine shipping. The system considers various intensity levels of bioaccumulation, living resource damage, risk to man (two categories), and effects on "amenities." The procedure is in a preliminary stage and under active revision. It illustrates the problem of scales or systems that group data and establish arbitrary (i.e., fixed) score classes; there are five fixed nonhuman toxicity classes and five for human LD_{50}. In our view, this represents a limitation of some proposed hazard profiles wherein data must be placed into a few restricted consideration categories.

Oller *et al.* (1980) described a procedure for a surveillance index construction which has quantitative aspects.

The U. S. Environmental Protection Agency[2] listed 10 factors to be considered in revising the 307a toxic substances list. These include toxicity, persistence, bioconcentration, synergistic effect, water solubility, extent of point source discharges, potential human exposure, annual production and use patterns, and detectability. A later revision used a reduced set of four attributes and attempted to relate these by use of the simple additive formula

$$H = O + B + P \cdot T,$$

[2] *Fed. Reg.* **44,** 18279, March 17, 1979.

where relative hazard potential (H) was viewed as a function of occurrence (O), bioaccumulation (B), the product of persistence (P), and toxicity (T).

The International Register of Potentially Toxic Chemicals (Huismans, 1980) began an effort to identify the attributes or characteristics of internationally used substances to evaluate potential hazards of these chemicals. The list of attributes considered 17 major categories and about 80 separate informational items (e.g., flash point, environmental pathway, spill history, etc.). The author notes (p. 379) that "a data profile . . . need not necessarily have data available on all attributes," thus illustrating the problem of completing all the required informational needs. Furthermore as of 1978, profiles had been produced for only 10 compounds. "New" compounds will be difficult to profile, and total assessments presumably must await data development.

Canton and Slooff (1979) recommend that a compound should be tested for toxicity, persistence, and bioaccumulation. They critique some past and some recent efforts to classify compounds and also argue for standardization. Ribeyre *et al.* (1979) reported on the difficulty of designing and implementing "trophic" multispecies bioassays. While the "meaningfulness" of the test is excellent, the "needed" test requirements to apply this more broadly are staggering and imply, if not a bleak future, efforts of a herculean nature. There simply does not appear to be enough time, personnel, or resources to address completely each new crop of compounds, let alone develop required data for existing entities. They thoughtfully define the problems to be addressed in developing "ecological test procedures" (pp. 424–425). Presumably, test results will be reproducible if care is exercised in using their procedures since variability among similar tests appears to be a problem. Gerike and Fischer (1979) have shown that, at least with a battery of biodegradation tests, the degree of biodegradation appears to be test specific, and Muller (1980) discusses variability in tests using *Daphnia*.

From our point of view, we lack procedures to estimate persistence that are simple, inexpensive, and meaningful. Presently techniques are lacking to utilize currently available or easily generated data as the primary point of departure. Although there appears to be no shortage of proposed test techniques, few workers actually deal with the process of assessment or the use of multifactor data in that context.

While the above is not intended to be a rigorous review of existing literature, it illustrates several problems:

(1) Most proposed methods or techniques require, advocate, or imply the generation of new data. The corollary to this is that small use is made of existing or easily acquired data which oftentimes represent the only information available.

(2) Many existing or proposed methods fail to deal with the assessment problem in truly quantitative or mathematical terms. Very few of the methods reduce the scope of consideration to a single value which can be used comparatively.

(3) Information categories (here termed "factors") range from simply physical–chemical concerns, such as vapor pressure and solubility, to highly complex items, such as ecological tests involving a number of trophic components. The most commonly encountered factors, however, are facets of toxicity, accumulation, and persistance. The methodology employed in the development of our index—an index

intended to reflect aquatic toxicological concerns—may have broader application to the community of workers dealing with similar problems.

CONCEPTUAL CONSIDERATIONS

Concepts and constructs used in this paper owe much to environmental quality index techniques summarized by Ott (1978) (see especially pp. 197–301). With some differences, the methods proposed in this paper are modeled after those used in developing the National Sanitation Foundation (NSF) Water Quality Index (Brown *et al.*, 1970; Landwehr, 1974). We consider the primary desirable features of an aquatic environmental index usage to be:

(1) normalization of a subindex scale to a known range of variability which includes some substances previously identified as hazardous (e.g., the bioaccumulation potential of DDT);
(2) expression of subindices and the composite index on scales which range from 0 to 100;
(3) computational techniques which allow the combination of disparate attributes, such as toxicity data, bioaccumulation potential, and persistence data, into a single index score;
(4) the potential to standardize vocabulary and procedures for aquatic toxicology;
(5) maximal systematic utilization of existing information through development of rating scales.

Below, we will illustrate the approach by use of a three-factor index based upon considerations of vertebrate and invertebrate acute toxicity data and bioaccumulation potential; fate data were not available. Factor selection is critical if evaluations are to have ecologic value—our example was influenced by availability of toxicity data and the ease and cost of producing minimal data sets necessary for index computation.

Our example employs two acute static toxicity tests and one physical–chemical procedure—factors optimized for aquatic toxicological concerns. Other factors could be exchanged for those used, and there is no real limit to the total number of factors which could be employed in constructing an index although three to seven attributes appears to be usual, at least in water quality application (Ott, 1978). Considerations, such as geographic use patterns of pesticide application or total quantity of a hazardous substance produced or applied, are potential factors for subindex scale selection. Subindex scales could be easily constructed, assuming the availability of quality data sets or the capability to generate such data sets.

SUBINDEX SCALE CONSTRUCTION

Johnson and Finley (1980) reported on toxicity testing conducted from 1965 to 1978 at the Columbia National Fisheries Research Laboratory. Over that period, more than 400 chemicals were used in acute toxicity tests on a wide variety of organisms. Chiefly, the organisms tested represented fish and invertebrate taxonomic groups, the latter because of their greater relative sensitivity to many com-

TABLE 1

CHEMICAL COMPOUNDS USED IN INDEX SCALE DEVELOPMENT

Compound	Acute toxicity (μg/l)		Octanol–water partition coefficient
	Invertebrate LC_{50}	Vertebrate LC_{50}	
Acephate	50,000	1,100,000	1.2
Aldrin	4,300	2.6	1,000,000
Carbaryl	26	1,950	230
Chlordane	40	42	1,000,000
DDT	1	8.7	960,000
Dichlobenil	11	140	559
Dichlorvos	0.5	170	25
Dieldrin	640	1.2	97,439
Diflubenzuron	30	240,000	7,680
Diuron	160	4,900	94
Endrin	4.3	.75	218,000
Ethion	1.8	500	23,092
Fenitrothion	3	2,400	2,400
Fenvalerate (Pydrin)*	0.021	120.9	1,584,000
Heptachlor	56	7.4	275,423
Kepone	180	30	207,395
Lindane	10	27	7,079
Malathion	0.76	200	780
Methomyl	1,050	1,200	2
Methyoxychlor	1.9	62	47,500
Mexacarbate	40	12.0	1,370
Nitralin	1,300	30,000	13,044
Paraquat	11,000	15,000	29,482
Parathion ethyl	1.3	1,430	6,400
Parathion methyl	3.8	3,700	82
Payoff (AC222,705)*	0.023	1.8	1,584,000
Permethrin*	0.046	88.4	3,162,000
2,4-D Phenoxy	3,800	21,300	37
2,4,5-T	50,000	900	4
Phosmet	2.0	400.0	677
Picloram	27	8,200	2
Propham	19	38	11
Ronnel	4,300	550	46 400
Simazine	100,000	100,000	155
Toxaphene	26	10.6	797,787
Trichlorfon	40	1,750	3
Trifluralin	2,200	41	220,000

Note. Except for asterisked items, all toxicity data are from Johnson and Finley (1980). Octanol–water data are from various sources (see references). Asterisked items were supplied by Patrick Borthwick, U. S. Environmental Protection Agency, Environmental Research Laboratory, Gulf Breeze, Fla.

pounds. A subset of 34 compounds (Table 1) was selected to illustrate subindex scale construction. Octanol–water partition data were obtained from Kenaga (1980), Kenaga and Goring (1980), Konemann (1980), Leonard *et al.* (1976), McDuffie (1981), Neely *et al.* (1974), and Veith *et al.* (1979).

Additionally, in order to ensure that the subindex scale would adequately cover

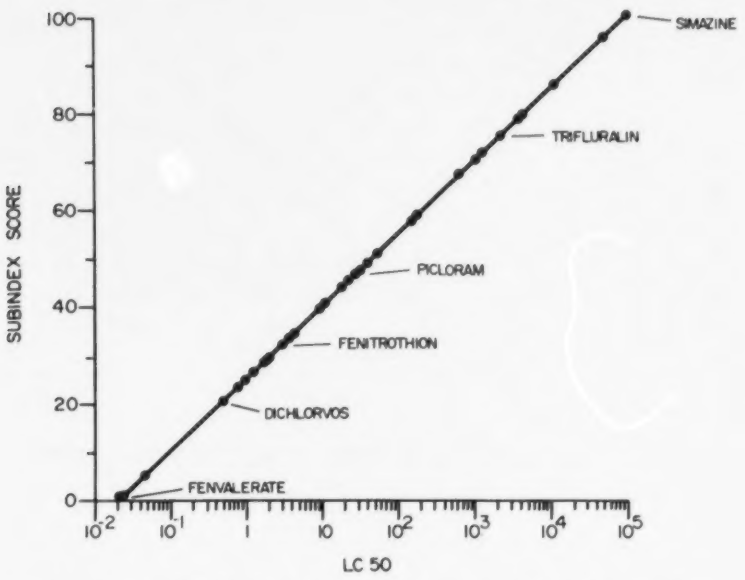

FIG. 1. Subindex scale for invertebrate LC_{50} ($\mu g/l$) toxicity factor. Only selected compounds are indicated. See Tables 1 and 2 for actual data and compound sequence.

the range for compounds that may have extremely low toxicity values, three data sets were added to the list of 34 compounds. These compounds asterisked in Table 1, are from unpublished acute tests on marine species.[3] The effect of this addition on the subindex scale was to extend the low range by several orders of magnitude. Except for these three compounds, selection criteria included test data on both Gammarid and Salmonid species; limitation to these taxonomic groups was intended to reduce variability due to interspecific differences. In selecting these substances, a conscious effort was made to select representatives of the following general classes of chemical insecticides: organophosphates, organochlorines, urea compounds, and pyrethroids.

Other selection criteria included an attempt to select representative compounds currently available and historically used as well as an attempt to include the probable maximum factor range from highest to lowest. We intend our index to reflect the comparative hazard of known and newly developed chemical compounds to aquatic organisms.

For each of the factors (invertebrate and vertebrate toxicity and octanol–water partition coefficient), chemicals were ranked to establish the range of the factor. The highest (and lowest) value determined the range of each subindex scale and a construction line was drawn from the highest (or lowest) value through the origin, with log of concentration plotted on the abscissa and a one-to-one hundred scale plotted on the ordinate (see Figs. 1–3). To ensure that all ordinate scales maintained

[3] Personal communication (1981): Patrick Borthwick, U. S. Environmental Protection Agency, Environmental Research Laboratory, Gulf Breeze, Fla. 32561. Species used were *Mysidopsis bahia* and *Cyprinodon variegatus*.

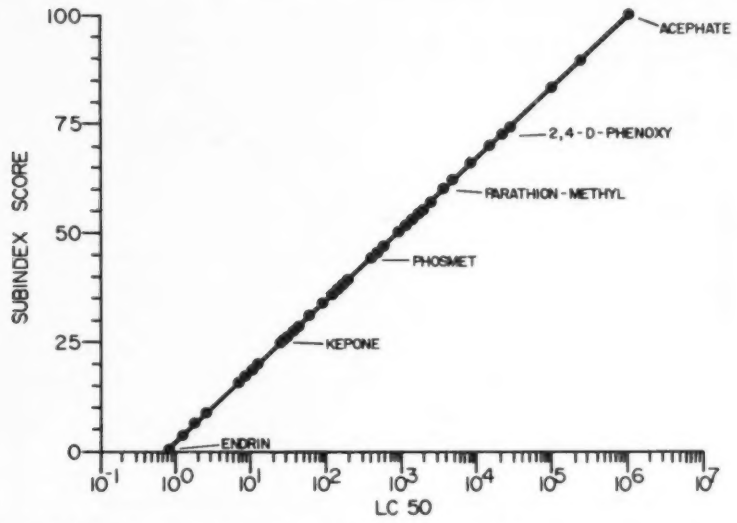

FIG. 2. Subindex scale for vertebrate LC_{50} ($\mu g/l$) toxicity factor. Only selected compounds are indicated. See Tables 1 and 2 for actual data and compound sequence.

the same desired relationship, octanol–water data were intentionally inverted to produce a decreasing series. In factor scale development, it is important to ensure that all variables either increase or decrease simultaneously; otherwise, aggregation procedures—the combination of subindex scores into a single index value—would cause subindex scores to cancel each other.

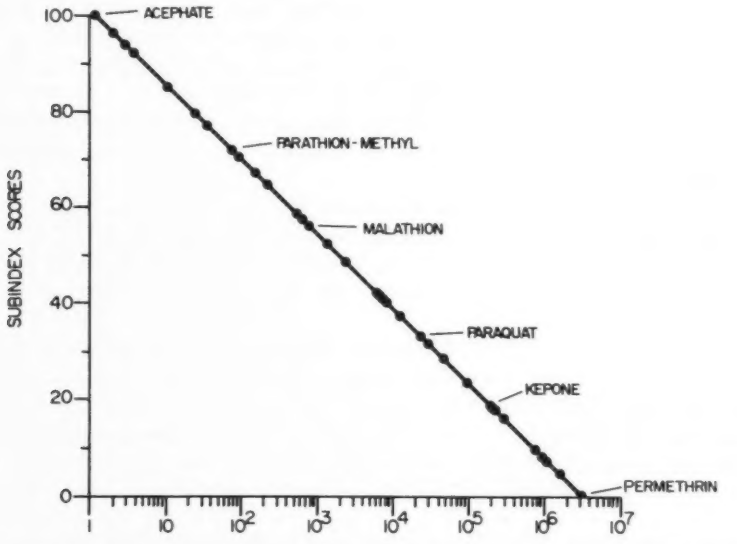

FIG. 3. Subindex scale for octanol–water partition data. Only selected compounds are indicated. See Tables 1 and 2 for actual data and compound sequence.

At this stage, a subindex score can be compared to those for known compounds. Also, the series of compounds of concern can be ordered according to the specific factor of concern (e.g., acute toxicity to an invertebrate species, etc.) with a numerical value that ranges from 0 to 100 (see Figs. 1–3). In effect, unknowns based on test results can be scaled to the factor range of known compounds and their relative ranking expressed over a fixed range of 0 to 100. There are many potential uses for such data. Obviously, other factors can be dealt with in the same manner, and it is important to emphasize that indices containing more than three factors can be easily constructed.

INDEX COMPUTATION

The process of compositing individual factor scores into a single index score is straightforward. This process, the aggregation step, closely parallels procedures used for the multiplicative form of the NSF water quality index (Brown *et al.*, 1970). Essentially, each subindex score is raised to a power and the result multiplied by each index term. Care should be taken to preserve each term by substituting some small positive value other than zero when subindex scores are very low. This allows a solution that would otherwise not be possible if an individual term goes to zero. Numerically, the process is described as

$$I_T = I_I^{0.33} I_F^{0.33} I_{OW}^{0.33}$$

where I_T is the total index, and I_I, I_F, and I_{OW} refer to the scaled subindex scores for invertebrate toxicity (I), fish toxicity (F), and octanol–water partition coefficients (OW). Insisting that the exponents sum to 1 ensures that the range of I_T will also be 0 to 100. Other exponential values could be employed, the only restriction being that all exponents used must sum to 1.

In our example, all exponents are equal; however, this is not necessary if there is a pragmatic basis for assigning other values. Varying exponents for a specific series has the effect of weighting an individual term. For example, if 0.50, 0.25, and 0.25, respectively, were used in the above computational (aggregation) formula, it would have the effect of weighting the invertebrate subindex twice as much as the other terms. Variable weighting, commonly used in index application, usually derives from a belief of greater relative importance for a given factor.

We illustrate I_T computation for DDT as follows:

	I_I Invertebrate	I_F Vertebrate	I_{OW} Octanol:water
Raw data (from Table 1)	1.0 μg/liter	8.7 μg/liter	960,000
Scaled date (from Figs. 1–3)	25.1	17.3	8.1

$I_T = (25.1)^{0.33}\ (17.3)^{0.33}\ (8.1)^{0.33} = 2.9 \times 2.6 \times 2.0 = 15.2 = I_T$ for DDT

Similar computation for all compounds listed in Table 1 produced the data for I_T given in Table 2.

TABLE 2

SCALED SUBINDEX AND TOTAL INDEX VALUES FOR CHEMICALS LISTED IN TABLE 1

Compound	I_I	I_F	I_{OW}	I_T
Acephate	95.5	100.0	100.0	98.5
Simazine	100.0	83.1	67.1	82.3
2,4,5-T	95.5	49.9	91.9	75.9
2,4-D Phenoxy	78.7	72.2	76.8	75.9
Methomyl	70.4	52.0	96.5	70.7
Picloram	46.6	65.5	96.5	66.5
Diuron	58.1	61.9	70.5	63.3
Trichlorfon	49.1	54.6	93.8	63.1
Nitralin	71.8	74.6	37.1	58.4
Paraquat	85.6	69.7	31.6	57.4
Diflubenzuron	47.2	89.3	40.7	55.6
Carbaryl	46.3	55.4	64.5	54.9
Parathion methyl	33.8	59.9	71.4	52.5
Ronnel	79.5	46.5	28.5	47.3
Propham	44.3	27.6	85.0	47.0
Fenitrothion	32.3	56.8	48.6	44.7
Dichlobenil	40.7	36.8	58.4	44.4
Phosmet	29.6	44.2	57.1	42.2
Dichlorvos	20.6	38.2	79.5	39.7
Parathion ethyl	26.8	53.2	42.0	39.1
Malathion	23.3	39.3	56.2	37.2
Mexacarbate	49.1	19.5	52.4	36.9
Ethion	28.9	45.8	33.3	35.3
Lindane	40.1	25.2	41.3	34.7
Trifluralin	75.2	28.2	18.0	33.7
Kepone	58.9	26.0	18.4	30.4
Methyoxychlor	29.3	31.1	28.4	29.6
Heptachlor	51.3	16.1	16.5	23.9
Chlordane	49.1	28.4	7.8	22.1
Toxaphene	46.3	18.7	9.3	20.0
Aldrin	79.5	8.8	7.8	17.6
Dieldrin	67.1	3.3	23.5	17.4
DDT	25.1	17.3	8.1	15.2
Payoff (AC222,705)	0.6	6.2	4.7	2.6
Endrin	34.6	0.0*	18.1	0.1
Fenvalerate (Pydrin)	0.0*	35.8	4.7	0.1
Permethrin	5.1	33.6	0.0*	0.1

Note. Subindex scale data for I_I, I_F, and I_{OW} are also shown in Figs. 1, 2, and 3, respectively. Total index computation procedure is given in the text. Asterisked scores are actually very small positive numbers (see data in Table 1).

DISCUSSION

As stated previously, this technique for obtaining a preliminary hazard assessment does not preclude testing and assessment protocols necessary to provide more definitive information on environmental impact. Indeed, interpretation of the meaning of the index score will still require informed and intuitive considerations. However, the index provides a quantitative technique for estimating and comparing the relative toxicological potential of chemicals.

For many compounds, considerable additional data exist beyond those needed to compute the three-factor index. Such factors as chronic toxicity tests, ecological and microcosm tests, environmental monitoring data, structure–activity information, etc., can be correlated or associated with both the subindex or total index data. Such comparisons might have important application with chemicals for which minimal laboratory data are available. Other important possibilities include the comparison of selected compounds in specific contexts, such as index rank-order difference of freshwater vs saltwater data sets and retrospective analyses of index statistics to evaluate possible chemical structural relationships.

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